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Discrete Schrödinger-Poisson Systems Preserving Energy and Mass

C. RINGHOFER*
Erwin Schrödinger Institut, Vienna, Austria
ringhofer@asu.edu

J. SOLER†
Departamento de Matemática Aplicada, Facultad de Ciencias
Universidad de Granada, 18071-Granada, Spain
jsoler@goliat.ugr.es

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Abstract—A discrete predictor-corrector Schrödinger-Poisson system is proposed which has the property of mass and energy conservation exactly on the discrete level. The discretization is based on the Cranck-Nicholson scheme, which preserves these invariants of the Schrödinger-Poisson system, but involves the solution of nonlinear equations at each time step. A modified linearized scheme is proposed where conservation is achieved by introducing a phase modulation in the corrector step.

1. INTRODUCTION

In many applications, it is necessary to compute the quantum mechanical evolution of an ensemble of particles over long periods of time. This involves the solution of the effective one particle Schrödinger equation obtained from a mean field approximation using Coulomb potentials [1], i.e., the Schrödinger-Poisson problem

$$i\hbar \frac{\partial \psi}{\partial t} + \frac{\hbar^2}{2m} \Delta_x \psi + \theta V \psi = 0, \tag{1.1a}$$

$$\Delta_x V = n, \tag{1.1b}$$

for the wave function $\psi(x,t)$ and the potential $V(x,t)$, where $n(x,t) = |\psi(x,t)|^2$ is the expected particle density for a pure quantum state in the position space $\mathbb{R}^3$ at the time t. Here units are assumed in which the mass of the particles equals m and $\theta = 1$ holds in the case of attracting forces and $\theta = -1$ holds in the case of repulsive forces. In the absence of boundary conditions (i.e., for the open quantum system or for systems in a periodic structure), there is a given set

*Permanent address: Department of Mathematics, Arizona State University, Tempe, AZ 85287 U.S.A.
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of integral invariants which are conserved for all time [2]. Indeed, there are eleven constants of motion: the mass M, the energy E, the linear momentum $\vec{P}$, the angular momentum $\vec{J}$, and the boost operator (generator of the pure Galilei transformations) $\vec{K}$ that form a closed algebra, isomorphic to the Lie algebra of the generators of the Galilei group, with the norm functional M playing the role of the inertial mass of the particle. When a discretization of the system is necessary, it will be important to preserve most of these invariants through the discretization. For example, if the radially symmetric case is considered, it is a simple matter to check that the conservation of angular momentum, linear momentum, and boost holds and it is possible to concentrate the efforts in preserving another invariant. However, the practically most important usually are the mass of particles, given in terms of the expected particle density, and the total energy, in terms of $1/2(\hbar^2/m|\nabla\psi|^2 - \theta V|\psi|^2)$. So

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^3} |\psi(x,t)|^2\,dx = 0, \tag{1.2a}$$

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^3} \frac{1}{2}\left[\frac{\hbar^2}{m}|\nabla\psi|^2 - \theta V|\psi|^2\right](x,t)\,dx = 0 \tag{1.2b}$$

holds [2]. Any stable and consistent discretization of the Schrödinger-Poisson system (1.1a),(1.1b) will retain the conservation property (1.2a),(1.2b), approximately up to the order of the discretization error. However, if (1.1a),(1.1b) are to be solved over long time intervals, it is desirable that (1.2a),(1.2b) hold *exactly* for the discretized system because discretization errors in the conservation laws (1.1a),(1.1b) will accumulate. As it turns out, it is relatively easy to satisfy (1.2a), but not so trivial to satisfy (1.2b) at the same time. In this paper, we present a predictor-corrector discretization of the Schrödinger-Poisson system (1.1a),(1.1b) which preserves mass as well as energy exactly on the discrete level. The scheme is formulated as an approximation to the Cranck-Nicholson scheme, which possesses the desired conservation properties, but involves the solution of nonlinear systems at each time step. The conservation of energy (1.2b) is achieved by modulating the phase of the corrector step by a term which is of the same order in Δt as the local discretization error. However, this modulation is only possible if the wave function ψ is neither purely real nor purely imaginary. The final result is therefore a hybrid scheme which requires the solution of nonlinear equations only for those time steps for which either the real or the imaginary part of ψ becomes too small.

The importance of obtaining a discrete system preserving mass and energy is motivated by the sensitivity as opposed to the variations of the energy when trying to gain some insight into the quantum mechanical dynamics of a single particle in a vacuum or a polar crystal; i.e., the polaron problem. This is the case, for example, when the existence of so-called *breathing* mode solutions (changing size oscillatory wave functions) is investigated in the case of attractive potentials with negative energy. The existence of these periodic solutions is a consequence of a minimizing variational principle with constraints, involving the energy. Therefore, the control of the energy in the discrete model will be relevant, see [2].

Finally, let us remark that the existence and uniqueness of solutions that justify the approximations made in this paper have been analyzed in [3,4].

2. THE SPATIAL DISCRETIZATION

We will first define the finite difference discretization of the Laplace operator. This discretization will be of a quite general form but has to satisfy the appropriate identities for the discrete equivalent of integration by parts. We define an arbitrarily structured mesh $X = \{\mathbf{x}_m : m = 1, 2, \dots\}$ on which the discrete approximation of the wave function ψ is defined. The approximation of the gradient of the wave function is then defined on the dual mesh $Y = \{\mathbf{y}_n : n = 1, 2, \dots\}$. Usually, the dual mesh Y will consist of the midpoints of edges connecting two neighboring grid

points of the X-mesh. We define the discrete approximation of the L^2 product of variables given on these meshes by

$$\langle u, v\rangle_X := \sum_{m\in\mathbb{N}} \alpha_m u^*(\mathbf{x}_m)v(\mathbf{x}_m), \qquad \langle U, W\rangle_Y := \sum_{n\in\mathbb{N}} U(\mathbf{y}_n)^H A_n W(\mathbf{y}_n), \tag{2.1}$$

for some integration weights α_m and A_n, where the A_n will, in general, be real symmetric positive definite matrices. (Here "$*$" denotes the complex conjugate and "H" denotes the Hermitian of a complex vector.) Now let the discrete gradient of a grid function u be defined by some vector valued finite difference coefficients D_{mn}. Then we define the discrete divergence of a vector valued grid function U by its dual operator with respect to the inner product (2.1). Therefore,

$$\nabla_D u(\mathbf{y}_n) := \sum_{m\in\mathbb{N}} D_{nm}u(\mathbf{x}_m), \tag{2.2a}$$

$$\operatorname{div}_D U(\mathbf{x}_m) := -\sum_{n\in\mathbb{N}} \frac{1}{\alpha_m} D_{nm}^T A_n U(\mathbf{y}_n) \tag{2.2b}$$

holds. With this definition, $\langle u, \operatorname{div}_D W\rangle_X = -\langle \nabla_D u, W\rangle_Y$ holds. Other than the validity of this discrete Gauss theorem, we will make no further use of the structure of the spatial discretization in this paper. The spatially discretized Schrödinger-Poisson system is now given by

$$i\hbar\frac{\partial\psi}{\partial t} + \frac{\hbar^2}{2m}\Delta_D\psi + \theta V\psi = 0, \tag{2.3a}$$

$$\Delta_D V = |\psi|^2, \tag{2.3b}$$

$$\Delta_D := \operatorname{div}_D \nabla_D. \tag{2.3c}$$

3. THE CRANCK-NICHOLSON SCHEME

We now proceed to show that, if the semidiscrete system (2.3a)–(2.3c) is discretized by the Cranck-Nicholson scheme (or the trapezoidal rule) in the time direction, mass as well as energy is preserved exactly on the discrete level. Of course, using the trapezoidal rule implies solving a nonlinear system of equations at each time step, which will, in general, be too computationally expensive. However, this conservation property will be important in the next section where the nonlinear system is approximated by a predictor-corrector approach. In general, we approximate a grid function u on the discrete time level t_k by u^k, and define the time differencing and averaging operators δ_t and μ_t by

$$\delta_t u^k = \frac{1}{\Delta t_k}\left(u^{k+1} - u^k\right), \qquad \mu_t u^k = \frac{1}{2}\left(u^{k+1} + u^k\right). \tag{3.1}$$

Note that if the spatial mesh (and therefore, the coefficients D_{mn} in (2.2a),(2.2b)) is independent of time, the temporal operators δ_t, μ_t commute with the spatial operators $\nabla_D, \operatorname{div}_D, \Delta_D$. The Cranck-Nicholson discretization of the Schrödinger-Poisson system now reads

$$i\hbar\delta_t\psi + \frac{\hbar^2}{2}\mu_t\Delta_D\psi + \theta(\mu_t V)(\mu_t\psi) = 0, \tag{3.2a}$$

$$\Delta_D V = |\psi|^2. \tag{3.2b}$$

To prove the mass and energy conservation properties of the scheme (3.2a),(3.2b), we need the easily verified identities

$$\delta_t(uw) = (\mu_t u)(\delta_t w) + (\delta_t u)(\mu_t w), \qquad \delta_t\left(|u|^2\right) = 2\operatorname{Re}\left[(\mu_t u^*)\,(\delta_t u)\right]. \tag{3.3}$$

In order to derive the mass conservation property, we take the inner product of (3.2a) with $i\mu_t\psi$ and take the real part. This gives, for each of the terms in (3.2a),

$$2\,\mathrm{Re}\langle(\mu_t\psi),(\delta_t\psi)\rangle_X = \delta_t\|\psi\|_X^2, \tag{3.4a}$$

$$2\,\mathrm{Re}\langle i(\mu_t\psi)(\mu_t\Delta_D\psi)\rangle_X = 2\,\mathrm{Re}\left[i\langle(\mu_t\nabla_D\psi),(\mu_t\nabla_D\psi)\rangle_Y\right] = 0, \tag{3.4b}$$

$$2\,\mathrm{Re}\langle i(\mu_t\psi),(\mu_t V)(\mu_t\psi)\rangle_X = 2\,\mathrm{Re}\left[-i\left\langle(\mu_t V),|\mu_t\psi|^2\right\rangle_X\right] = 0, \tag{3.4c}$$

where we write $\|\psi\|_X^2$ for $\langle\psi,\psi\rangle_X$. Thus, (3.4a)–(3.4c), gives the discrete mass conservation law $\delta_t\|\psi\|_X^2 = 0$. To show the energy conservation property, we multiply (3.2a) by $-\delta_t\psi$ and again take the real part. We obtain for each term

$$2\,\mathrm{Re}\langle-\delta_t\psi, i\delta_t\psi\rangle_X = 2\,\mathrm{Re}\left[-i\|\delta_t\psi\|_X^2\right] = 0, \tag{3.5a}$$

$$2\,\mathrm{Re}\langle-\delta_t\psi,\mu_t\Delta_D\psi\rangle_X = 2\,\mathrm{Re}\langle\delta_t\nabla_D\psi,\mu_t\nabla_D\psi\rangle_Y = \delta_t\|\nabla_D\psi\|_Y^2, \tag{3.5b}$$

$$\begin{aligned} 2\,\mathrm{Re}\langle-\delta_t\psi,(\mu_t V)(\mu_t\psi)\rangle_X &= -\left\langle(\mu_t V),2\,\mathrm{Re}\left[(\delta_t\psi)^*(\mu_t\psi)\right]\right\rangle_X = -\left\langle(\mu_t V),\delta_t|\psi|^2\right\rangle_X \\ &= -\langle(\mu_t V),\delta_t\Delta_D V\rangle_X = \langle(\mu_t\nabla_D V),\delta_t\nabla_D V\rangle_Y \\ &= -\frac{1}{2}\langle(\mu_t V),\delta_t\Delta_D V\rangle_X - \frac{1}{2}\langle(\mu_t\Delta_D V),\delta_t V\rangle_X \\ &= -\frac{1}{2}\delta_t\langle V,\Delta_D V\rangle_X = -\frac{1}{2}\delta_t\left\langle V,|\psi|^2\right\rangle_X. \end{aligned} \tag{3.5c}$$

Adding up the estimates in (3.5a)–(3.5c), gives the energy conservation equation

$$\delta_t\left[\hbar^2\|\nabla_D\psi\|_Y^2 - \theta\left\langle V,|\psi|^2\right\rangle_X\right] = 0. \tag{3.6}$$

Note that if we had discretized the nonlinear term $V\psi$ in (2.3a) by the midpoint rule (i.e., by $\mu_t(V\psi)$ instead of $\mu_t V\mu_t\psi$), energy would not be preserved exactly at each time step.

4. THE PREDICTOR-CORRECTOR SCHEME

We now proceed to approximate the second-order accurate Cranck-Nicholson scheme of the previous section, which requires the solution of the nonlinear system of equations (3.2a),(3.2b), for ψ^{k+1}, V^{k+1} at each time step, by a predictor-corrector scheme of the same order, requiring only the solution of linear equations at each step. One step of the predictor corrector scheme will be of the form $\psi^k \to \psi^{k,1} \to \psi^{k,2} \to \psi^{k+1}$, where $\psi^{k,1}, \psi^{k,2}$ denote the intermediate stages of the scheme. To this end, we define the stage-time differencing and averaging operators $\delta_t^{(1)}, \mu_t^{(1)}, \delta_t^{(2)}, \mu_t^{(2)}$ by $\delta_t^{(1)}u^k = (1/\Delta t_k)(u^{k,1} - u^k)$, etc. Given ψ^k, the predictor step is then given by

$$i\hbar\delta_t^{(1)}\psi^k + \frac{\hbar^2}{2}\mu_t^{(1)}\Delta_D\psi^k + \theta V^k\left(\mu_t^{(1)}\psi^k\right) = 0, \tag{4.1a}$$

$$\Delta_D V^{k,1} = \left|\psi^{k,1}\right|^2. \tag{4.1b}$$

Note that, since the term $\mu_t V$ in (3.2a) has been replaced by V^k in (4.1a), this represents two decoupled linear equations for $\psi^{k,1}$ and $V^{k,1}$. The standard corrector step is now given by

$$i\hbar\delta_t^{(2)}\psi^k + \frac{\hbar^2}{2}\mu_t^{(2)}\Delta_D\psi^k + \theta\left(\mu_t^{(1)}V^k\right)\left(\mu_t^{(2)}\psi^k\right) = 0, \tag{4.2a}$$

$$\Delta_D V^{k,2} = \left|\psi^{k,2}\right|^2. \tag{4.2b}$$

Again, this represents two decoupled linear systems for $\psi^{k,2}, V^{k,2}$ since $V^{k,1}$ and $(\mu_t^{(1)}V^k)$ are known at this stage. It is easily verified that scheme (4.1a)–(4.2b) is second-order consistent in time. As in Section 3, discrete mass conservation is verified by computing as in (3.4a)–(3.4c), the

real part of the inner product of (4.2a) with $i\mu_t^{(2)}\psi$, which gives $\delta_t^{(2)}\|\psi\|_X^2 = 0$. Thus, the obvious predictor corrector approach preserves mass. To investigate the energy conservation properties of (4.1a)–(4.2b), we multiply (4.2a) by $-\delta_t^{(2)}\psi$ and obtain for the first two terms as before,

$$2\,\mathrm{Re}\left\langle -\delta_t^{(2)}\psi, i\delta_t^{(2)}\psi\right\rangle_X = 0, \qquad 2\,\mathrm{Re}\left\langle -\delta_t^{(2)}\psi, \mu_t^{(2)}\Delta_D\psi\right\rangle_X = \delta_t^{(2)}\|\nabla_D\psi\|_Y^2. \tag{4.3}$$

The third term in (4.2a), we write as a correction to the nonlinear Cranck-Nicholson scheme and obtain

$$\begin{aligned} &2\,\mathrm{Re}\left\langle -\delta_t^{(2)}\psi, \left(\mu_t^{(1)}V\right)\left(\mu_t^{(2)}\psi\right)\right\rangle_X \\ &= 2\,\mathrm{Re}\left\langle -\delta_t^{(2)}\psi, \left(\mu_t^{(2)}V\right)\left(\mu_t^{(2)}\psi\right)\right\rangle_X + 2\,\mathrm{Re}\left\langle \delta_t^{(2)}\psi, \frac{1}{2}\left(V^{k,2}-V^{k,1}\right)\left(\mu_t^{(2)}\psi\right)\right\rangle_X. \end{aligned} \tag{4.4}$$

Proceeding as in (3.5c), we obtain for the first term on the right-hand side of (4.4),

$$2\,\mathrm{Re}\left\langle -\delta_t^{(2)}\psi, \left(\mu_t^{(2)}V\right)\left(\mu_t^{(2)}\psi\right)\right\rangle_X = -\frac{1}{2}\,\delta_t^{(2)}\left\langle V, |\psi|^2\right\rangle_X. \tag{4.5}$$

For the second term on the right-hand side of (4.4), we obtain

$$\begin{aligned} &2\,\mathrm{Re}\left\langle \delta_t^{(2)}\psi, \frac{1}{2}\left(V^{k,2}-V^{k,1}\right)\left(\mu_t^{(2)}\psi\right)\right\rangle_X \\ &= \left\langle \frac{1}{2}\left(V^{k,2}-V^{k,1}\right), 2\,\mathrm{Re}\left[\left(\delta_t^{(2)}\psi^*\right)\left(\mu_t^{(2)}\psi\right)\right]\right\rangle_X = \frac{1}{2}\left\langle \left(V^{k,2}-V^{k,1}\right), \delta_t^{(2)}|\psi|^2\right\rangle_X. \end{aligned} \tag{4.6}$$

Combining (4.3)–(4.6), we obtain the evolution of the total discrete energy as

$$\delta_t^{(2)}\left[\hbar^2\|\nabla_D\psi\|_Y^2 - \theta\left\langle V, |\psi|^2\right\rangle_X\right] = \theta\left\langle \left(V^{k,1}-V^{k,2}\right), \delta_t^{(2)}|\psi|^2\right\rangle_X. \tag{4.7}$$

Therefore, the straight forward predictor-corrector approximation to the Cranck-Nicholson scheme preserves mass, but exhibits a spurious gain/loss of the total energy which is of order Δt^3 at each time step. (Taylor expansion easily verifies that $V^{k,1} - V^{k,2} = O(\Delta t^2)$ holds.) We remedy this situation by modulating the phase of the second stage $\psi^{k,2}$ of the scheme, setting $\psi^{k+1}(\mathbf{x}_m) = \psi^{k,2}(\mathbf{x}_m)\exp[i\Delta t_k^3\omega g(\mathbf{x}_m)]$, where ω is a real parameter and g is some real function bounded uniformly in $\mathbf{x}$. Obviously, this correction does not change the absolute value of $\psi^{k,2}$, and therefore, the mass conservation property is retained. Also, adding an order $O(\Delta_t^3)$ correction at each step does not destroy the overall second-order accuracy of the method. Using this correction, (4.7) becomes

$$\left[\hbar^2\|\nabla_D\psi\|_Y^2 - \theta\left\langle V, |\psi|^2\right\rangle_X\right]^{k+1} = \left[\hbar^2\|\nabla_D\psi\|_Y^2 - \theta\left\langle V, |\psi|^2\right\rangle_X\right]^k + R, \tag{4.8a}$$

$$R = \hbar^2\left(\|\nabla_D\psi^{k+1}\|_Y^2 - \|\nabla_D\psi^{k,2}\|_Y^2\right) + \Delta t_k\theta\left\langle \left(V^{k,1}-V^{k,2}\right), \delta_t^{(2)}|\psi|^2\right\rangle_X, \tag{4.8b}$$

$$V^{k+1} = V^{k,2}. \tag{4.8c}$$

The parameter ω is now chosen such that the residual R in (4.8a) vanishes identically. This involves the solution of a single scalar nonlinear equation for ω. In leading order in Δt_k, the parameter ω is given by

$$\omega = \frac{\theta\left\langle V^{k,2}-V^{k,1}, \delta_t^{(2)}|\psi|^2\right\rangle_X}{2\hbar^2\Delta t_k^2\,\mathrm{Re}\left\langle i\nabla_D\left(g\psi^{k,2}\right), \nabla_D\psi^{k,2}\right\rangle} + O(\Delta t_k). \tag{4.9}$$

Note that the denominator in (4.9) becomes zero if either the real or the imaginary part of the wave function $\psi^{k,2}$ vanishes identically. In this case, the modulation strategy breaks down, since

the parameter ω can become arbitrarily large and the corrector loses its consistency. For those time steps for which either the real or the imaginary part of ψ becomes too small, one therefore has to revert to the full nonlinear Cranck-Nicholson scheme of the previous section. However, this will be a rather rare event, and solving the full nonlinear system (3.2a),(3.2b), occasionally represents an acceptable computational cost. On the other hand, if the wave function ψ is neither purely real nor purely imaginary, the denominator in (4.9) can always be made nonzero by choosing an appropriate modulation function g and (4.9) can be used as an initial guess for a (scalar) Newton iteration to determine ω.

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